1.0

1.1

1.25   1.4

4.5
5.0
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The problem of hot carrier diffusion in semiconductors is studied with a non-Markovian Retarded Langevin Equation (RLE) applied to the case of carriers in the transient dynamic response (TDR) to a steady homogeneous electric field. A non-stationary velocity fluctuation/correlation function is defined and related to a time dependent diffusion coefficient. This is applied to n-type silicon and the parameters of interest are studied as a function of space and/ or time. The problem of non-stationary diffusion is particularly important in very short channel devices in which TDR and velocity overshoot occur.

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NON-EQUILIBRIUM HOT-CARRIER DIFFUSION PHENOMENON IN SEMICONDUCTORS
1. A THEORETICAL NON-MARKOVIAN APPROACH[+]

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Résumé - Le problème de la diffusion de porteurs chauds dans les semicon-
ducteurs est étudié à l'aide d'une Equation de Langevin Retardée (RLE)
appliquée au cas de la réponse transitoire dynamique (TDR) à un champ électrique
stationnaire homogène. Une fonction de corrélation des fluctuations de vitesse
non-stationnaire est définie et est reliée à un coéfficient de diffusion
dépendant du temps. Ceci est appliqué au Silicium type-N et les quantités
intéressantes sont étudiées en fonction de l'espace et/ou du temps. Le
problème de diffusion non-stationnaire est particulièrement important dans
les composants à canaux ultra-courts où réponse transitoire dynamique et sur-
vitesse se manifestent.

Abstract - The problem of hot carrier diffusion in semiconductors is studied
with a non-Markovian Retarded Langevin Equation (RLE) applied to the case of
carriers in the transient dynamic response (TDR) to a steady homogeneous elec-
tric field. A non-stationary velocity fluctuation/correlation function is
defined and related to a time dependent diffusion coefficient. This is applied
to n-type silicon and the parameters of interest are studied as a function of
space and/or time. The problem of non-stationary diffusion is particularly
important in very short channel devices in which TDR and velocity overshoot
occur.

1. **Introduction.-** In recent years, much interest has centered upon the transient
dynamic response of electrons as it impacts carrier transport through small spatial
regions of high electric field. With recent improvements in technological fabrica-
tion of very-short-channel devices, this problem has become not only of theoretical
interest but of practical interest as well. For instance, in the pinch-off region
of a short-gate field-effect transistor, the carriers injected at the source move
by a combination of drift and diffusion in a very high electric field. Then the
transit time of the carriers under the gate can be shorter than, or of the same
order of magnitude as, the time needed to establish a steady-state high-field dis-
tribution function. In fact, a condition for this to occur is that the transit-
time in the high-field region be comparable to the momentum relaxation time thus
causing the velocity to increase, but much shorter than the energy relaxation time.
Thus, on average the carriers may transit through a considerable portion of the
high-field region with almost their low field mobility even though the applied
field corresponds to the saturated velocity range [1]. This is true not only for
the first-order moment of the distribution function of the carriers (drift velocity),
but also is true for higher order moments, and especially for diffusion (related to
the second moment). The diffusion coefficient is one of the most important

parameters required in modeling semiconductor devices, it is not only necessary for
evaluating operating characteristics and frequency characteristics but it provides
also fundamental characterization of velocity fluctuations in the system and their
contribution to noise in the device [2]. Diffusion actually is a process depending
upon velocity correlation and the relationship between diffusion and drift, as
expressed by the Einstein relation, is a steady-state relation [3]. Indeed, tract-
able results for the steady-state hot electron problem have only recently been
achieved [4-6]. The problem in the transient region is complicated by the fact that
the random-walk equations governing transient diffusion do not reduce to normal
Fick's law behavior on time scales comparable to the relaxation process, a result of
the general non-Markovian and non-stationary nature of transport on these time
scales. In this paper, we address some of these problems with the help of a Retard-
ed Langevin Equation (RLE) in order to approach the random walk of the carriers.
Furthermore, we define a non-stationary two-time correlation function for the ve-
locity fluctuations which can be related to a transient diffusion coefficient. The
formal solution of the RLE allows us to derive a general expression for the correla-
tion function. Then, we deal with the diffusion coefficient itself and show in
particular that the transient diffusion coefficient is related to the time deriva-
tive of the mean-square displacement of the carriers. However, it is found that in
the limit of long times, stationarity and the normal equations for correlation and
diffusion are recovered.

2. The Retarded Langevin Equation Approach.- We consider an ensemble of carriers
initially at equilibrium with the crystal lattice. The ensemble is represented by
a Maxwell-Boltzmann distribution in v-space ($<v> = 0$ and $<v^2> = 3k_BT_L/m$ with T_L the
lattice temperature). At a certain time, referred as $t = o$, we apply a macroscopi-
cally homogeneous and steady electric field whose amplitude corresponds to hot car-
riers. These conditions give rise to a TDR regime in which the system relaxes toward
a non-equilibrium, steady-state and often exhibits a velocity overshoot.

The motion of the particles is governed by a Retarded Langevin Equation for the
velocity of the carriers, and is written as [7,8]

$$m \frac{dv}{dt} = -m \int_0^t \dot{\gamma}(t-u) \, v(u)du + R(t) + qE_o h(t) \quad , \tag{1}$$

where $R(t)$ is a random force symbolizing the random (non-regular) part of the col-
lisions of the carriers with the lattice (no carrier-carrier interaction is consid-
ered here), E_o is the external field, and $h(t)$ is the Heavyside function. $\dot{\gamma}(t)$ is
the memory function of the system and is related to the correlation function of the
total force applied to the system. For instance in the case of a stationary regime,
we would have $\dot{\gamma}(t) = <R(o)R(t)>/m^2<v^2(o)>$, in absence of external forces [3].

Equation (1) is a non-Markovian form of the Langevin equation, since the rate
of change of the velocity at t not only depends on the velocity at that time but
also depends on all past time. Further, it is a non-stationary equation, since the

lower bound in the integral refers to that time where the disturbing field was applied. It is generally admitted by now that only an equation such as (1) can describe very-fast processes [3,7,8], and in particular the TDR regime can be described in this way. In (1), we have assumed a parabolic energy band [9].

We may easily solve (1) using Laplace transforms. We introduce a function $X(t)$ defined by its Laplace transform, as

$$\hat{X}(s) = (s + \hat{\gamma}(s))^{-1} \quad . \tag{2}$$

Then, coming back to time domain, we find

$$v(t) = v(o)X(t) + \frac{qE_o}{m} \int_0^t X(u)du + \frac{1}{m} \int_0^t R(t-u) \, X(u)du \quad , \tag{3}$$

which is a general expression of the evolution of the velocity of each carrier under the influence of the external field and of the collisions. We get $X(t)$ by averaging (3) over the ensemble (we assume $\langle R(t) \rangle = 0$). The result is

$$X(t) = \frac{m}{qE_o} \frac{dv_d}{dt} \quad , \tag{4}$$

where $v_d(t)$ is the ensemble drift velocity of the carriers. Therefore $X(t)$ represents in fact the macroscopic acceleration of the ensemble. However $X(t)$ can be given another definition. We define a non-stationary correlation function for the velocity fluctuations as

$$\phi_{\Delta v}(t',t) = \phi_{\Delta v}(t,t') = \langle v(t)v(t') \rangle - v_d(t)v_d(t') \quad . \tag{5}$$

Multiplying both sides of (1) by $v(o)$, averaging over the ensemble (note that $\langle R(t)v(o) \rangle = 0$), Laplace transforming and making use of (2) we obtain after re-transforming

$$\phi_{\Delta v}(o,t) = \langle v^2(o) \rangle \, X(t) \quad . \tag{6}$$

$X(t)$ is the reduced non-stationary correlation function calculated at $t' = o$. Comparing this equality with (4) gives

$$v_d(t) = \frac{qE_o}{m\langle v^2(o) \rangle} \int_0^t \phi_{\Delta v}(o,t')dt' \quad . \tag{7}$$

This relationship existing between the first and a second moment of the velocities of the carriers is a direct intrinsic property of the NLE used to describe the TDR regime. Whether this equality is met is one of the goals of the next paper [10], but (7) is a statement of the familiar Kubo formula [11] found in equilibrium statistical mechanics.

To develop a complete expression for the correlation function defined in (5), we need to know the correlation function of the random force $R(t)$ which appears when we put (3) into (5). If we assume that the collisions occur instantaneously in time we can write

$$\langle R(t)R(t')\rangle = 2\pi I_R(t,t')\delta(|t-t'|) \tag{8}$$

Relaxation of this condition does not significantly affect the results found in the present work. A consequence of (8) is that only $I_{R1}(t) = I_R(t,t'=t)$ is of interest in the current context and this latter function can be obtained from the time evolution of the mean energy of the ensemble. Then the correlation function $\phi_{\Delta v}$ can be put in the form (with $\theta \geq 0$)

$$\phi_{\Delta v}(t_o, t_o + \theta) = \langle v^2(o)\rangle X(t_o)X(t_o + \theta) + \frac{2\pi}{m^2}\int_0^{t_o} I_{R1}(t_o-y)X(y)X(y + \theta)dy \quad , \tag{9}$$

and in particular we obtain for the mean-energy:

$$\langle \varepsilon(t)\rangle = \frac{1}{2} m\, v_d^2(t) + \frac{1}{2} m \langle v^2(o)\rangle X^2(t) + \frac{\pi}{m}\int_0^t I_{R1}(t-y)\, X^2(y)dy \quad . \tag{10}$$

We can sum up this part by saying that if, in the current conditions of the TDR regime, the evolutions of the drift velocity and the mean-energy are known, then the fluctuations of the system are completely specified through (9) and (10) together with (4).

3. The Diffusion Coefficient.- Using expression (5) for the non-stationary correlation function of velocity fluctuations, we can define a non-stationary or time-dependent diffusion coefficient, which is a generalization of the definition given in a stationary regime [3,6]:

$$D(t) = \int_0^t \phi_{\Delta v}(t',t)dt' \quad . \tag{11}$$

Another way to define the diffusion is through the spreading of a packet of carriers drifting under the influence of the external force and spreading due to the fluctuations of the velocities of the carriers. This spreading is characterized by the mean-square displacement of the carriers starting from a known initial distribution (a Dirac-function in space, for instance). It is easy to see that

$$\langle \Delta x^2(t)\rangle = \langle (x(t)-\langle x(t)\rangle)^2\rangle = \int_0^t \int_0^t \phi_{\Delta v}(t',t'')dt'dt'' \quad . \tag{12}$$

From the definition (12), it is straightforward to show that

$$\frac{1}{2}\frac{d}{dt}\langle \Delta x^2(t)\rangle = \int_0^t \phi_{\Delta v}(t',t)dt' = D(t) \quad . \tag{13}$$

This shows that the diffusion coefficient defined in (11) is related to the time-derivative of the average-square displacement. The usual definition of the diffusion in a steady-state is in fact a limiting case of relation (13). When the time t' at which the integration of $\phi_{\Delta v}(t',t)$ begins is greater than the time t_s needed for the system to reach stationarity, $\phi_{\Delta v}$ becomes an even function of $t-t'$ only, then

$$\frac{1}{2}\frac{d}{dt}\langle \Delta x^2(t)\rangle = \int_0^{t \geq t_s} \phi_{\Delta v}(\eta)d\eta = D_s(t) \tag{14}$$

As $t \to \infty$, $D_s(t)$ tends to a constant finite limit D_s and

$$\lim_{t \to \infty} <\Delta x^2(t)> = 2t \, D_s \tag{15}$$

Therefore (11) defines a general diffusion coefficient which is valid in both stationary and non-stationary regimes, and as we did above for $\phi_{\Delta v}$ we can derive an expression for $<\Delta x^2(t)>$:

$$<\Delta x^2(t)> = \frac{m^2}{q^2 E_o^2} <v^2(o)> v_d^2(t) + \frac{2\pi}{q^2 E_o^2} \int_o^t I_{R1}(t-u) \, v_d^2(u) du \quad . \tag{16}$$

The expression of $D(t)$ follows immediately using (13).

4. Application and Discussion.- In the case of n-type Si<111>, the carriers behave as if the energy band was unique with an isotropic effective mass m . There, the concepts described above are easily applied.

i) The oscillatory nature of the velocity overshoot strongly suggests that the memory function $\gamma(t)$ (and $\dot{\gamma}(t)$, as well) is an exponential. So we specify $\gamma(t)$ via the ansatz [12]

$$\gamma(t) = [\gamma_o + a(1 - e^{-\Gamma t})]h(t) \quad , \tag{17}$$

$1/\Gamma$ is the time needed for the system to reach stationarity and as such is equivalent to the energy relaxation time.

ii) To have an insight into the time dependence of $I_{R1}(t)$, we can make use of (10) and the results given by a Monte Carlo method [10] for $<\epsilon(t)>$. It is thus possible to show that

$$I_{R1}(t) = I_{Ro} + (I_{R\infty} - I_{Ro})(1 - e^{-\Gamma_o t}) \quad , \quad \Gamma_o \simeq \Gamma \tag{18}$$

is a good approximation for the correlation function of the random force R(t). $I_{R\infty}$ is given by the static diffusion coefficient

$$D_s = \frac{\pi I_{R\infty}}{m^2(a + \gamma_o)^2} \quad , \tag{19}$$

and $I_{Ro} << I_{R\infty}$. The value of I_{Ro} does not affect significantly the results since at short times the second term in the RHS of (16) is an order of magnitude smaller than the first term.

Taking (17) and (18) into account, $\phi_{\Delta v}(t',t)$ and $D(t)$ are easily derived analytically and computed. We present here some computed results obtained with $E = 50$ kV/cm. The non-stationary correlation function is displayed in Fig. 1, and its evolution is studied for different initial times t_o from 0 to 0.5 ps (the latter corresponds to the steady-state). The fact that the correlation function is steeper when t_o is longer can be explained by the increase of the scattering frequency as a function of time corresponding to the heating of the carriers. In other words, at short times the correlation function is dominated by the initial distribution of the velocities of the carriers, while at longer times, when the steady-state is

approached, the system has been completely randomized by the collisions and the correlation function is dominated by the random force (i.e. $I_{R1}(t)$).

The mean-square displacement and diffusion coefficient are displayed in Fig. 2 as a function of the distance travelled by the carriers. This shows the spatial extension over which the system is in a non-stationary regime, ~ 400 Å in the present case. These results are compared to what would occur in case of a pure ballistic regime. In fact, the calculated D(x) departs from the ballistic trend even at very short times (and distances) meaning that no ballistic regime exists for transient diffusion. On the contrary at longer times D(x) goes through a maximum and then decreases to its stationary value. This is, of course, related to the oscillatory nature of the correlation functions and these oscillations are essentially the consequence of the combination of momentum and energy relaxation in the resolvent $\tilde{X}(s)$ of the RLE. In the present example, this resolvent is a rational fraction which has two complex conjugate poles.

Possible extensions of the work could be: i) the application of the present technique to multivalley semiconductors; ii) to take into account spatial variations of the electric field and then get a more precise picture of what occurs in a short-channel device; iii) to try a more physical and less phenomenological approach using quantum statistical mechanics [13].

In summary, we have obtained here a consistent definition of the diffusion coefficient in terms of the velocity auto-correlation function. This definition is valid in the transient and non-stationary regime and reduces to the normal expression as steady-state is approached. The application of this to the retarded, non-stationary Langevin equation yields expressions for the velocity correlation function and diffusion coefficient which have excellent qualitative agreement and satisfactory quantitative agreement to results obtained by a Monte Carlo method [10].

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the momentum $p(t)$ instead of the velocity $v(t)$, and the formula $v(t) = p(t)$ $(1 + 2\alpha p^2(t)/m_o)^{-1/2}/m_o$ for example. In this case, the derivations would be much more involved.

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12. Y_o is the inverse momentum relaxation time at thermal equilibrium and $a + Y_o$ is the inverse momentum relaxation time when non-equilibrium steady-state is reached.

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Figure 1.
Transient Reduced Correlation
Functions Calculated At
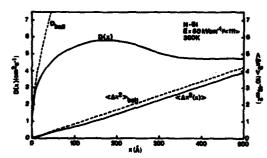$t_o=0$(___);$t_o=0.02$ps(---);$t_o=0.5$ps(-.-)

Figure 2.
Mean-Square Displacement (right scale)
and Diffusion Coefficient (left scale)
as a Function of Distance. Dashed
Curves Stand for a Pure Ballistic
Trend